Quantum-chemical study of protonated forms of vanillic acid in electronically excited states

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The vanillic acid is important to study because it is used as a catalyst in the isomerization reaction to produce polymers and pharmaceuticals. The vanillic acid structure of these compounds is the presence in their structures of oxygen reactive groups: methoxy, hydroxyl and carboxyl. Its are leading to a large variety of photophysical and photochemical processes occurring in them during excitation electromagnetic field.

In work using quantum chemical methods [1]: CHPDP / s (partial neglect of differential overlap with spectroscopic parameterization) and IRENA (molecular electrostatic potential) an analysis of possible ways of deactivation of electronically excited states of 4-hydroxy-3-methoxy-benzoic acid (vanillic acid) and its protolytic forms were studied. The ratio of radiative and non-radiative deactivation constants of channels of electronic excitation energy were established. The rate constants of photophysical processes (internal and intersystem crossing), occurring after the absorption of light in these forms have been received.

1. N.Yu. Vasil'eva, O.V. Vusovich, N.M. Kozhevnikova. High Energy Chemistry. 2002. T. **36**. № 4. C. 265-271.